Exploring the Potential of Quasi-One-Dimensional Organic Crystals of TTT_2I_3 for Thermoelectric Applications

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Abstract. This paper estimates the potential of using quasi-one-dimensional organic crystals of TTT_2I_3 (tetrathiotetracene-iodide) as prospective thermoelectric converters. A comprehensive physical model of the crystal was developed and numerical calculations were performed based on the derived analytical expressions. Along with the free hole and phonon energies and the impurity scattering term, the main Hamiltonian of the physical model incorporates two types of hole-phonon interactions: the first interaction involves the deformation potential and the second interaction characterized by polaron effects. Charge transport along the TTT chains is of band-type, while charge transport between the neighboring molecules in different molecular chains is of the hopping type. The electrical conductivity, Seebeck coefficient, thermal conductivity, thermoelectric power factor and figure of merit were calculated as functions of charge carrier concentrations, temperature and impurity concentration. A detailed analysis of the charge-lattice interaction, including the investigation of the Peierls structural transition in the TTT molecular chains of TTT_2I_3, was carried out, leading to the

determination of the critical transition temperature. Additionally, considering the random phase approximation, the dispersion law of renormalized phonons was examined at different temperatures for two cases: one including interaction between TTT chains, and another where this interaction is neglected.

References

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